

Tris(2-hydroxyethyl) isocyanurate
839-90-7 | DTXSID4026266

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.82e-09 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.86e-01

Confidence level: 3.59e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Thiourea</div> <div>Measured: 1.50e-08</div> <div>Predicted: 2.26e-03</div>	<div>Image not found</div> <div>Sevoflurane</div> <div>Measured: 2.48e-08</div> <div>Predicted: 264</div>	<div>Image not found</div> <div>2,6-Dichlorodiphenyl ether</div> <div>Measured: 3.60e-06</div> <div>Predicted: 9.64e-04</div>
<div>Image not found</div> <div>4-Chloro-3-methylphenol</div> <div>Measured: 1.50e-12</div> <div>Predicted: 5.35e-02</div>	<div>Image not found</div> <div>L-Glutamic acid</div> <div>Measured: 1.70e-08</div> <div>Predicted: 1.68e-08</div>	